QD Algorithms and Algebraic Eigenvalue Problems

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ABSTRACT

A sketch of the standard *QD* algorithm is followed by the derivation of two similar algorithms for the calculation of all the eigenvalues of the matrix A from the sequence $\{A^r\mathbf{g}_0\}$. The existence of one of the methods is established and bounds for the results are given when A is totally positive. The paper concludes by showing the close connection between the *QD* algorithm for the calculation of the zeros of a polynomial and the method of treppeniteration for the calculation of the eigenvalues of its companion matrix.

1. INTRODUCTION

It is a standard result in elementary algebra that the general solution of the recurrence $a_0u_{r+2}+a_1u_{r+1}+a_2u_r=0$ is given by $u_r=A_1\alpha_1^r+A_2\alpha_2^r$, where α_1 and α_2 are the zeros (supposed unequal for simplicity) of the quadratic $a_0z^2+a_1z+a_2$. Thus when u_0 and u_{-1} are prescribed, u_n is easily found. Alternatively this can be used to provide a method for finding the larger zero in modulus of the quadratic, for we can write

$$\frac{u_{r+1}}{u_r}=\alpha_1\frac{A_1+A_2(\alpha_2/\alpha_1)^{r+1}}{A_1+A_2(\alpha_2/\alpha_1)^r},$$

and so if $|\alpha_2|<|\alpha_1|$ and $A_1\neq 0$, then $u_{r+1}/u_r\to\alpha_1$ as $r\to\infty$. This is Bernoulli's method for the calculation of the dominant zero of a quadratic and can clearly be extended to a method for finding the dominant zero, if it exists, of a polynomial of arbitrary degree.

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It is natural to ask if it can be extended to solve the problem of finding repeated or complex dominant zeros, and perhaps even to finding all the zeros. Aitken [1] gave a partial answer, and Rutishauser [9] gave a complete generalization, which is known as the QD algorithm.

In order to motivate some of this paper and set the notation we shall outline the background to the theory. This will be very restricted in scope; for a comprehensive account reference should be made to Henrici [5].

The problem is that of calculating the zeros of the polynomial

$$a_0 z^n + a_1 z^{n-1} + \cdots + a_{n-1} z + a_n; \tag{1.1}$$

to this end define the sequence $\{u_r\}$ by

$$a_0 u_{r+n} + a_1 u_{r+n-1} + \cdots + a_{n-1} u_{r+1} + a_n u_r = 0, \qquad r = 1-n, 2-n, \ldots, \tag{1.2a}$$

with

$$u_0 = 1, \qquad u_{-1} = u_{-2} = \cdots = u_{-n+1} = 0. \tag{1.2b}$$

Other starting conditions can be used, but these are convenient. It can be shown that if the zeros are $\alpha_1, \alpha_2, \ldots, \alpha_n$ and if they satisfy

$$|\alpha_1| > |\alpha_2| > \cdots > |\alpha_n| > 0, \tag{1.3}$$

then the general solution of (1.2) is given by

$$u_r = \sum_{k=1}^{n} A_k \alpha_k^r. \tag{1.4}$$

The algorithm depends on properties of the Hankel determinants

$$H_r^{(k)} = \begin{vmatrix} u_r & u_{r+1} & \cdots & u_{r+k-1} \\ u_{r+1} & u_{r+2} & \cdots & u_{r+k} \\ \vdots & \vdots & & \vdots \\ u_{r+k-1} & u_{r+k} & \cdots & u_{r+2k-2} \end{vmatrix}, \qquad r = 1, 2, \ldots, \quad k = 1, 2, \ldots, n. \tag{1.5}$$

It is not difficult to show with the aid of the representation (1.4) and the Binet-Cauchy theorem that

$$H_r^{(k)} \sim (\alpha_1\alpha_2\cdots\alpha_k)^r \quad \text{as } r\to\infty, \qquad k=1,2,\ldots,n;$$

consequently

$$\frac{H_{r+1}^{(k)}}{H_r^{(k)}} \to \alpha_1\alpha_2\cdots\alpha_k \qquad \text{as} \quad r\to\infty. \tag{1.6}$$

Let

$$q_r^{(k)} = \frac{H_{r+1}^{(k)}}{H_r^{(k)}} \Big/ \frac{H_{r+1}^{(k-1)}}{H_r^{(k-1)}}; \tag{1.7}$$

then, from (1.6), we see that

$$q_r^{(k)} \to \alpha_k \qquad \text{as} \quad r\to\infty. \tag{1.8}$$

The problem of calculating α_k now becomes that of calculating the sequence $\{q_r^{(k)}\}$ and its limit. This is the problem which Rutishauser solved with the aid of the identity

$$H_{r-1}^{(k)}H_{r+1}^{(k)} - H_{r-1}^{(k+1)}H_{r+1}^{(k-1)} = \left[H_r^{(k)}\right]^2 \tag{1.9}$$

as follows. Let

$$e_r^{(k)} = \frac{H_r^{(k+1)}}{H_{r+1}^{(k)}}\,\frac{H_{r+1}^{(k-1)}}{H_r^{(k)}}; \tag{1.10}$$

then it is not difficult to show that

$$e_r^{(k)} \to 0 \qquad \text{as} \quad r\to\infty. \tag{1.11}$$

Moreover, the following quotient-difference relations hold:

$$\begin{aligned} q_r^{(k+1)} &= q_{r+1}^{(k)}e_{r+1}^{(k)}/e_r^{(k)}, \\ e_r^{(k)} &= e_{r+1}^{(k-1)} + q_{r+1}^{(k)} - q_r^{(k)}. \end{aligned} \tag{1.12}$$

These relations provide a simple algorithm whereby $\{q_r^{(k)}\}$ can be calculated for $k = 1,2,\ldots,n$. This is more clearly presented in the form of the QD array

$$
\begin{array}{ccccc}
 & q_0^{(1)} & & & \\
e_0^{(0)} & & e_0^{(1)} & & \\
 & q_1^{(1)} & & q_0^{(2)} & \\
e_1^{(0)} & & e_1^{(1)} & & e_0^{(2)} \\
 & q_2^{(1)} & \div & q_1^{(2)} & \\
e_2^{(0)} & & e_2^{(1)} & - & e_1^{(2)} \\
 & q_3^{(1)} & & q_2^{(2)} &
\end{array}
$$

The algorithm is started with $e_r^{(0)} = 0$, $r = 0, 1, \ldots,$ and $q_r^{(1)} = u_{r+1}/u_r$, and succeeding columns are calculated with the aid of (1.12).

The algorithm can also be used to calculate zeros of power series. The form in which it is presented here is numerically unstable. Fortunately however there is a stable form; details will be found in [5].

The basic ingredients of the QD algorithm are clearly the Hankel determinants, their asymptotic properties, and the relationship between them.

The remainder of this paper is in two distinct parts, both however being rooted the QD algorithm. In the first part we shall give an algorithm similar to the QD algorithm for the calculation of all the eigenvalues of a matrix and show that for totally positive matrices the scheme will provide upper and lower bounds for its eigenvalues. These latter results were suggested by those in Perfect [8], and indeed the whole of this part was stimulated by that paper.

In the second part we shall give a partial answer to a question of Moler [7]. This stems from the observation that the zeros of a polynomial are the eigenvalues of any of its companion matrices. Moler suggested that perhaps one should solve this eigenvalue problem in order to find the zeros of the polynomial. We shall show the close connection between the QD algorithm, treppeniteration, and Rutishauser's LR algorithm in this situation.

2. THE MATRIX EIGENVALUE PROBLEM

Let A be an $n \times n$ matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ which satisfy

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n| > 0. \tag{2.1}$$

This assumption is made for simplicity of presentation. The theory given here could be adapted to cover the situation when A has repeated eigenvalues, but it is felt that the extra complication is not worthwhile.

Essentially the question which will be posed is whether it is possible to calculate all the eigenvalues from the sequence of vectors $\{\mathbf{g}_r\}$, defined by

$$\mathbf{g}_{r+1} = A\mathbf{g}_r, \qquad r = 0, 1, \ldots, \tag{2.2}$$

where $\mathbf{g}_0$ is arbitrary. This iteration forms the basis of the power method for finding the dominant eigenvalue, and we shall see that in certain circumstances it carries all the information needed to calculate all the eigenvalues.

Unfortunately there will be a considerable amount of algebra in the following, and to avoid too many suffixes we shall write

$$\mathbf{g}_r = [g_r(1), g_r(2), \ldots, g_r(n)]^T.$$

We prove first a result concerning an analogue of the Hankel determinant which is suitable in this case.

Lemma 1. *Let*

$$D_r(i_1, i_2, \ldots, i_p) = \begin{vmatrix} g_r(i_1) & g_r(i_2) & \cdots & g_r(i_p) \\ g_{r+1}(i_1) & g_{r+1}(i_2) & \cdots & g_{r+1}(i_p) \\ \vdots & \vdots & & \vdots \\ g_{r+p-1}(i_1) & g_{r+p-1}(i_2) & \cdots & g_{r+p-1}(i_p) \end{vmatrix}.$$

Then, if the quotients are defined,

$$\lim_{r \to \infty} \frac{D_{r+1}}{D_r}(i_1, i_2, \ldots, i_p) = \lambda_1 \lambda_2 \cdots \lambda_p, \qquad 1 \leqslant p \leqslant n.$$

Proof. Since A has distinct eigenvalues, its eigenvectors $\{\mathbf{u}_s\}$ form a basis, and so we can write

$$\mathbf{g}_0 = \sum_{s=1}^{n} p_s \mathbf{u}_s;$$

consequently

$$\mathbf{g}_r = \sum_{s=1}^{n} p_s \lambda_s^r \mathbf{u}_s.$$

It follows that

$$g_r(i) = \sum_{s=1}^{n} p_s \lambda_s^r u_s(i), \qquad i = 1, 2, \ldots, n.$$

The use of this representation together with the Binet-Cauchy theorem will give the required result, exactly as in the proof of the corresponding result in the *QD* algorithm. ■

We note however that the result may not hold if the original choice of $\mathbf{g}_0$ was unfortunate (cf. the situation in the normal power method, where A_1 may vanish); however, in practice rounding errors in the arithmetic would militate against this. Furthermore some denominators may vanish; it would be possible to give conditions under which this will not happen, but it is simpler to take the naive viewpoint of ignoring the results up to that point and to take a new starting vector.

To complete the analogy with Rutishauser's algorithm we require a Hankel identity; this is provided by the following lemma.

LEMMA 2.

$$\begin{vmatrix} b_{11} & \cdots & b_{1m} \\ \vdots & & \vdots \\ b_{m1} & \cdots & b_{mm} \end{vmatrix} \begin{vmatrix} b_{22} & \cdots & b_{2m+1} \\ \vdots & & \vdots \\ b_{m+12} & \cdots & b_{m+1m+1} \end{vmatrix}$$

$$- \begin{vmatrix} b_{21} & \cdots & b_{2m} \\ \vdots & & \vdots \\ b_{m+11} & \cdots & b_{m+1m} \end{vmatrix} \begin{vmatrix} b_{12} & \cdots & b_{1m+1} \\ \vdots & & \vdots \\ b_{m2} & \cdots & b_{mm+1} \end{vmatrix}$$

$$= \begin{vmatrix} b_{22} & \cdots & b_{2m} \\ \vdots & & \vdots \\ b_{m2} & \cdots & b_{mm} \end{vmatrix} \begin{vmatrix} b_{11} & \cdots & b_{1m+1} \\ \vdots & & \vdots \\ b_{m+11} & \cdots & b_{m+1m+1} \end{vmatrix}.$$

Proof. In the larger determinant on the right hand side, take the first and last columns and rows as pivotal in Sylvester's identity. The result is almost immediate. See Gantmakher [3] or Karlin [6]. ■

COROLLARY.

$$D_r(i+1,\ldots,i+p)\cdot D_{r+1}(i+2,\ldots,i+p+1)$$
$$-D_{r+1}(i+1,\ldots,i+p)D_r(i+2,\ldots,i+p+1)$$
$$=D_{r+1}(i+2,\ldots,i+p)\cdot D_r(i+1,\ldots,i+p+1).$$

Proof. Set $m=p+1$ and $b_{jk}=g_{r+j-1}(i+k)$ in the identity. ■

This lemma allows us to define two QD schemes:

Scheme 1. For $0 \leqslant i \leqslant n-p$, let

$$q_r(i+1,\ldots,i+p)=\frac{D_{r+1}(i+1,\ldots,i+p)}{D_r(i+1,\ldots,i+p)}\frac{D_r(i+2,\ldots,i+p)}{D_{r+1}(i+2,\ldots,i+p)}$$

and

$$e_r(i+1,\ldots,i+p)=\frac{D_r(i+2,\ldots,i+p-1)}{D_r(i+1,\ldots,i+p-1)}\frac{D_r(i+1,\ldots,i+p)}{D_r(i+2,\ldots,i+p)}.$$

Then

$$\lim_{r\to\infty} q_r(i+1,\ldots,i+p)=\lambda_p$$

and

$$\lim_{r\to\infty} e_r(i+1,\ldots,i+p)=0.$$

Moreover the following quotient-difference relations hold:

$$\frac{q_r(i+1,\ldots,i+p+1)}{q_r(i+1,\ldots,i+p)}=\frac{e_{r+1}(i+1,\ldots,i+p+1)}{e_r(i+1,\ldots,i+p+1)},$$

$$q_r(i+2,\ldots,i+p+1)-q_r(i+1,\ldots,i+p)$$
$$=e_r(i+1,\ldots,i+p+1)-e_{r+1}(i+2,\ldots,i+p+1).$$

Scheme 2. For $0 \leqslant i \leqslant n-p$, let

$$Q_r(i+1,\ldots,i+p) = \frac{D_{r+1}(i+1,\ldots,i+p)}{D_r(i+1,\ldots,i+p)} \frac{D_r(i+2,\ldots,i+p)}{D_{r+1}(i+2,\ldots,i+p)}$$

and

$$E_r(i+1,\ldots,i+p) = \frac{D_r(i+2,\ldots,i+p-1)}{D_r(i+2,\ldots,i+p)} \frac{D_r(i+1,\ldots,i+p)}{D_r(i+1,\ldots,i+p-1)}.$$

Then

$$\lim_{r\to\infty} Q_r(i+1,\ldots,i+p) = \lambda_p, \qquad p = 1,2,\ldots,n,$$

and

$$\lim_{r\to\infty} E_r(i+1,\ldots,i+p) = 0, \qquad p = 1,2,\ldots,n.$$

The following relations are satisfied:

$$\frac{Q_r(i+1,\ldots,i+p)}{Q_r(i+2,\ldots,i+p)} = \frac{E_{r+1}(i+1,\ldots,i+p)}{E_r(i+1,\ldots,i+p)}$$

and

$$Q_r(i+2,\ldots,i+p+1) - Q_r(i+1,\ldots,i+p)$$
$$= E_r(i+1,\ldots,i+p+1) - E_{r+1}(i+1,\ldots,i+p).$$

We shall prove the results for scheme 1 only.

The convergence of $q_r(i+1,\ldots,i+p)$ to λ_p follows from Lemma 1, and since

$$D_r(i+1,\ldots,i+p) \sim (\lambda_1\lambda_2\cdots\lambda_p)^r \qquad \text{as} \quad r\to\infty,$$

we see that

$$e_r(i+1,\ldots,i+p) \sim \frac{(\lambda_1\cdots\lambda_{p-2})^r}{(\lambda_1\cdots\lambda_{p-1})^r} \frac{(\lambda_1\cdots\lambda_p)^r}{(\lambda_1\cdots\lambda_{p-1})^r}$$
$$= \left(\frac{\lambda_p}{\lambda_{p-1}}\right)^r.$$

Since by assumption $|\lambda_p/\lambda_{p-1}| < 1$, it follows that

$$e_r(i+1,\ldots,i+p) \to 0 \qquad \text{as} \quad r \to \infty.$$

The verification of the quotient part of the algorithm is immediate, and the difference part is not difficult to prove with the aid of the identity of the corollary to Lemma 2.

The schemes presented here are in a sense two dimensional ones, and for comparison with the usual *QD* array we present the one furnished by scheme 1:

$r = 1$:

$$\begin{array}{lllll}
q_1(1) & & & & \\
q_1(2) & e_1(1,2) & q_1(1,2) & & \\
q_1(3) & e_1(2,3) & q_1(2,3) & e_1(1,2,3) & \cdots \\
q_1(4) & e_1(3,4) & q_1(3,4) & e_1(2,3,4) & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{array}$$

$r = 2$:

$$\begin{array}{lllll}
q_2(1) & & & & \\
q_2(2) & e_2(1,2) & q_2(1,2) & & \\
q_2(3) & e_2(2,3) & q_2(2,3) & e_2(1,2,3) & \cdots \\
q_2(4) & e_2(3,4) & q_2(3,4) & e_2(2,3,4) & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{array}$$

$r = 3$:

$$\begin{array}{lllll}
q_3(1) & & & & \\
q_3(2) & e_3(1,2) & q_3(1,2) & & \\
q_3(3) & e_3(2,3) & q_3(2,3) & e_3(1,2,3) & \cdots \\
q_3(4) & e_3(3,4) & q_3(3,4) & e_3(2,3,4) & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{array}$$

In order to begin the algorithm we need to define $e_1(i+1) = 0$, $i = 0, 1, \ldots$. Then the first e-column can be calculated from the first q-column. However, the second q-column requires the values in the first e-column of the next iterate; for example

$$q_1(1,2) = q_1(1)e_2(1,2)/e_1(1,2).$$

Thus the table for $r=1$ can be completed only when $\mathbf{g}_{n+1}$ has been calculated.

Numerical example.

$$A=\begin{bmatrix} 14 & 14 & 6 & 1 \\ 14 & 20 & 15 & 6 \\ 6 & 15 & 20 & 14 \\ 1 & 6 & 14 & 14 \end{bmatrix},$$

The eigenvalues are 47.360678, 17.944271, 2.639320, 0.055728. The starting vector is $\mathbf{g}_0 = [14\ \ 14\ \ 6\ \ 1]^T$. The QD array is as follows:

$r=1$:

39.109557						
43.779720	4.670163	18.194086				
52.471962	8.692242	16.171905	1.188670	2.641462		
64.270408	11.798446	14.042995	1.028691	2.486882	0.003610	0.075366

$r=2$:

43.677733					
45.850331	2.172598	18.361210			
49.061181	3.210850	17.320825	0.172574	2.639263	
52.218782	3.157601	16.422081	0.158190	2.615479	0.000103

$r=3$:

45.853815			
46.767130	0.913315	18.147129	
47.980089	1.212959	17.712541	0.024806
49.037022	1.056933	17.354141	0.023887

$r=4$:

46.771346	
47.132800	0.361454
47.592195	0.459395
47.974482	0.382287

COMMENT. This is clearly an inefficient way to solve the eigenvalue problem. A more sensible numerical procedure based on the classical QD algorithm is given by Rutishauser in *Z. Angew. Math. Phys.* 5:496–508 (1954) and *Numer. Math.* 5:95–112 (1963). I am grateful to the referee for pointing out these references.

3. TOTALLY POSITIVE MATRICES

When the matrix A has only positive entries and $\mathbf{g}_0$ is a positive vector, then $\{\mathbf{g}_r\}$ will be composed of positive vectors. So in this case the successive quotients $g_r(i+1)/g_r(i)$ will always exist, and we can assert (because of the Perron-Frobenius theorem) that

$$q_r(i+1) \to \lambda_1 \qquad \text{as} \quad r \to \infty.$$

We now investigate a generalization of this situation when the matrix is *totally positive.*

DEFINITION. A matrix is totally positive if every minor of every order is positive.

An extensive treatment of such matrices will be found in Gantmakher and Krein [4]; see also Gantmakher [3] and Karlin [6]. For our purposes we need the following results:

1. If A is an $n \times n$ totally positive matrix, then its eigenvalues $\lambda_1, \dots, \lambda_n$ satisfy

$$\lambda_1 > \lambda_2 > \cdots > \lambda_n > 0.$$

2. Let $\mathbf{u}_r$ be the eigenvector which corresponds to λ_r; then any linear combination $\sum_{s=1}^{p} \alpha_s \mathbf{u}_s$ has no more than $r-1$ sign changes. This can be formalized by the statement that the determinants

$$\begin{vmatrix} u_1(i_1) & u_1(i_2) & \cdots & u_1(i_p) \\ u_2(i_1) & u_2(i_2) & \cdots & u_2(i_p) \\ \vdots & \vdots & & \vdots \\ u_p(i_1) & u_p(i_2) & \cdots & u_p(i_p) \end{vmatrix} > 0$$

for $1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$.

We shall show that the schemes will exist for totally positive matrices when $\mathbf{g}_0$ is taken to be the first column of A.

Before we embark on a proof of this and similar results it will be convenient to introduce a notation which will lessen the apparent complexity of the expressions: we define

$$A\begin{pmatrix} i_1, i_2, \dots, i_p \\ j_1, j_2, \dots, j_p \end{pmatrix} = \begin{vmatrix} a(i_1, j_1) & a(i_1, j_2) & \cdots & a(i_1, j_p) \\ a(i_2, j_1) & a(i_2, j_2) & \cdots & a(i_2, j_p) \\ \vdots & \vdots & & \vdots \\ a(i_p, j_1) & a(i_p, j_2) & \cdots & a(i_p, j_p) \end{vmatrix}.$$

LEMMA 3. *Let* $\mathbf{g}_0$ *be the first column of* A, *and* $\mathbf{g}_{r+1} = A\mathbf{g}_r$, $r = 0, 1, \dots$. *Then*

$$D_r(i_1, i_2, \dots, i_p) > 0 \quad \text{for} \quad 1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n, \qquad p = 1, 2, \dots, n.$$

Proof. We shall first prove by induction that

$$D_0(i_1, i_2, \dots, i_p) > 0 \quad \text{for } 1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n, \qquad p = 1, 2, \dots, n.$$

The result is clearly true for $p = 1$, since $D_0(i) = g_0(i) > 0$ by assumption.

Suppose that $D_0(j_1, j_2, \dots, j_{p-1}) > 0$ for $1 \leqslant j_1 < j_2 < \cdots < j_{p-1} \leqslant n$, and for $1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$ consider

$$D_0(i_1, i_2, \dots, i_p) = \begin{vmatrix} g_0(i_1) & g_0(i_2) & \cdots & g_0(i_p) \\ g_1(i_1) & g_1(i_2) & \cdots & g_1(i_p) \\ \vdots & \vdots & & \vdots \\ g_{p-1}(i_1) & g_{p-1}(i_2) & \cdots & g_{p-1}(i_p) \end{vmatrix}.$$

Now $\mathbf{g}_{r+1} = A\mathbf{g}_r$, $r = 0, 1, \dots$, and so this can be written as

$$\begin{vmatrix} a(i_1, 1) & a(i_2, 1) & \cdots & a(i_p, 1) \\ \sum_{j_1=1}^{n} a(i_1, j_1) g_0(j_1) & \sum_{j_1=1}^{n} a(i_2, j_1) g_0(j_1) & \cdots & \sum_{j_1=1}^{n} a(i_p, j_1) g_0(j_1) \\ \vdots & \vdots & & \vdots \\ \sum_{j_{p-1}=1}^{n} a(i_1, j_{p-1}) g_{p-2}(j_{p-1}) & \sum_{j_{p-1}=1}^{n} a(i_2, j_{p-1}) g_{p-2}(j_{p-1}) & \cdots & \sum_{j_{p-1}=1}^{n} a(i_p, j_{p-1}) g_{p-2}(j_{p-1}) \end{vmatrix}$$

$$= \sum_{j_{p-1}=1}^{n} \cdots \sum_{j_1=1}^{n} g_0(j_1) g_1(j_2) \cdots g_{p-2}(j_{p-1}) \begin{vmatrix} a(i_1, 1) & a(i_2, 1) & \cdots & a(i_p, 1) \\ a(i_1, j_1) & a(i_2, j_1) & \cdots & a(i_p, j_1) \\ \vdots & \vdots & & \vdots \\ a(i_1, j_{p-1}) & a(i_2, j_{p-1}) & \cdots & a(i_p, j_{p-1}) \end{vmatrix}$$

$$= \sum_{T_j} D_0(j_1, j_2, \dots, j_{p-1}) A\begin{pmatrix} i_1, i_2, \dots, i_p \\ 1, j_1, \dots, j_{p-1} \end{pmatrix},$$

where T_j is the index set which satisfies $1 \leqslant j_1 < j_2 < \cdots < j_{p-1} \leqslant n$.

Each product in this sum is positive, since its first element is positive because of the induction hypothesis and its second because A is totally positive.

The proof of the lemma will be completed by an induction on r as follows. Suppose that $D_r(j_1, j_2, \ldots, j_p) > 0$ for $1 \leqslant j_1 < \cdots < j_p \leqslant n$, and consider for $1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$ the determinant

$$D_{r+1}(i_1, i_2, \ldots, i_p)$$
$$= \begin{vmatrix} \sum_{j_1=1}^{n} a(i_1, j_1) g_r(j_1) & \cdots & \sum_{j_1=1}^{n} a(i_p, j_1) g_r(j_1) \\ \vdots & & \vdots \\ \sum_{j_p=1}^{n} a(i_1, j_p) g_{r+p-1}(j_p) & \cdots & \sum_{j_p=1}^{n} a(i_p, j_p) g_{r+p-1}(j_p) \end{vmatrix},$$

which, as above, can easily be seen to be

$$\sum_{T_j} D_r(j_1, j_2, \ldots, j_p) A\begin{pmatrix} i_1, i_2, \ldots, i_p \\ j_1, j_2, \ldots, j_p \end{pmatrix},$$

where T_j is the index set which satisfies $1 \leqslant j_1 < j_2 < \cdots < j_p \leqslant n$. As before, this sum is positive, and consequently the lemma is proved. ■

We note that the result can be interpreted as the statement that any linear combination of $\mathbf{g}_r, \mathbf{g}_{r+1}, \ldots, \mathbf{g}_{r+p-1}$ can have at most $p-1$ changes of sign in it.

Corollary. *If A is totally positive, then the QD schemes exist.*

Proof. The schemes exist if $D_r(i+1, \ldots, i+p)$ does not vanish for $r = 0, 1, 2, \ldots$ and $p = 1, 2, \ldots, n$, and this is a consequence of the lemma. ■

Lemma 4. *If A is totally positive, then for $p = 1, 2, \ldots, n$,*

$$\frac{D_{r+1}(1,2,\ldots,p)}{D_r(1,2,\ldots,p)} \leqslant \lambda_1 \lambda_2 \cdots \lambda_p \leqslant \frac{D_{r+1}(n-p+1,\ldots,n)}{D_r(n-p+1,\ldots,n)}$$

Proof. We shall show first that

$$\min \frac{D_{r+1}(i_1,i_2,\ldots,i_p)}{D_r(i_1,i_2,\ldots,i_p)} \leqslant \lambda_1\lambda_2\cdots\lambda_p \leqslant \max \frac{D_{r+1}(i_1,i_2,\ldots,i_p)}{D_r(i_1,i_2,\ldots,i_p)}$$

where the maximum and minimum are calculated over the range

$$1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n.$$

The total positivity of A clearly implies that of A^T, and so if $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_p$ are the eigenvectors of A^T corresponding to $\lambda_1, \lambda_2, \ldots, \lambda_p$ respectively, then

$$\begin{vmatrix} v_1(i_1) & v_1(i_2) & \cdots & v_1(i_p) \\ v_2(i_1) & v_2(i_2) & \cdots & v_2(i_p) \\ \vdots & \vdots & & \vdots \\ v_p(i_1) & v_p(i_2) & \cdots & v_p(i_p) \end{vmatrix} > 0$$

for $1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$. For simplicity denote this determinant by $V_p(i_1, i_2, \ldots, i_p)$.

Now since $A^T\mathbf{v}_s = \lambda_s\mathbf{v}_s$, we have

$$\lambda_1\lambda_2\cdots\lambda_p V_p(i_1,i_2,\ldots,i_p)$$

$$= \begin{vmatrix} \sum_{j_1=1}^{n} a(j_1,i_1)v_1(j_1) & \cdots & \sum_{j_1=1}^{n} a(j_1,i_p)v_1(j_1) \\ \vdots & & \vdots \\ \sum_{j_p=1}^{n} a(j_p,i_1)v_p(j_p) & \cdots & \sum_{j_p=1}^{n} a(j_p,i_p)v_p(j_p) \end{vmatrix}$$

$$= \sum_{j_1=1}^{n} \cdots \sum_{j_p=1}^{n} v_1(j_1)\cdots v_p(j_p) A\begin{pmatrix} j_1, j_2, \ldots, j_p \\ i_1, i_2, \ldots, i_p \end{pmatrix}$$

$$= \sum_{T_j} V_p(j_1, j_2, \ldots, j_p) A\begin{pmatrix} j_1, j_2, \ldots, j_p \\ i_1, i_2, \ldots, i_p \end{pmatrix}$$

where the summation is over $T_j: 1 \leqslant j_1 < j_2 < \cdots < j_p \leqslant n$. Multiply each side by $D_r(i_1, i_2, \ldots, i_p)$ and sum over $T_i: 1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$ to obtain

$$\lambda_1\lambda_2\cdots\lambda_p \sum_{T_i} V_p D_r(i_1, i_2, \ldots, i_p)$$

$$= \sum_{T_i} D_r(i_1, \ldots, i_p) \sum_{T_j} V_p(j_1, \ldots, j_p) A\begin{pmatrix} j_1 \cdots j_p \\ i_1 \cdots i_p \end{pmatrix}$$

$$= \sum_{T_j} V_p D_r(j_1, \ldots, j_p) \frac{\sum_{T_i} D_r(i_1, \ldots, i_p) A\begin{pmatrix} j_1 \cdots j_p \\ i_1 \cdots i_p \end{pmatrix}}{D_r(j_1, \ldots, j_p)}.$$

Hence $\lambda_1\lambda_2\cdots\lambda_p$ lies between the minimum and maximum over $1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$ of

$$\sum_{T_j} \frac{D_r(j_1, j_2, \ldots, j_p) A\begin{pmatrix} i_1, \ldots, i_p \\ j_1, \ldots, j_p \end{pmatrix}}{D_r(i_1, \ldots, i_p)}.$$

The summation can be expanded in the same fashion as it was contracted to give a summation over $1 \leqslant j_1, j_2, \ldots, j_p \leqslant n$, with the result that this quotient is $D_{r+1}(i_1, \ldots, i_p)/D_r(i_1, \ldots, i_p)$. (We note in passing that the full hypothesis that A is totally positive was not used here, and the result is true if only all the $p \times p$ minors are positive.)

Finally we shall show that if all the $(p+1)\times(p+1)$ minors are positive, then the extreme values lie at the end points as stated in the theorem. To this end note that the identity of Lemma 1 can be written

$$D_r(i_1, \ldots, i_p) D_{r+1}(i_2, \ldots, i_{p+1}) - D_{r+1}(i_1, \ldots, i_p) D_r(i_2, \ldots, i_p)$$
$$= D_{r+1}(i_2, \ldots, i_p) \cdot D_r(i_1, \ldots, i_{p+1}),$$

where

$$1 \leqslant i_1 < i_2 < \cdots < i_{p+1} \leqslant n,$$

and so

$$\frac{D_{r+1}}{D_r}(i_2, i_3, \ldots, i_{p+1}) - \frac{D_{r+1}}{D_r}(i_1, i_2, \ldots, i_p)$$
$$= \frac{D_{r+1}(i_2, \ldots, i_p) D_r(i_1, \ldots, i_{p+1})}{D_r(i_2, \ldots, i_{p+1}) D_r(i_1, \ldots, i_p)}.$$

We have shown that the right hand side is positive; consequently

$$\frac{D_{r+1}}{D_r}(i_2,\ldots,i_{p+1}) > \frac{D_{r+1}}{D_r}(i_1,i_2,\ldots,i_p).$$

Thus the maximum and minimum values of the quotients are attained at the ends, as stated. ■

The matrix in the example in Section 3 is totally positive, and it is easy to verify the truth of these results.

We next show that at each stage of the process the bounds improve.

LEMMA 5.

$$\min\frac{D_{r+1}(i_1,i_2,\ldots,i_p)}{D_r(i_1,i_2,\ldots,i_p)} < \min\frac{D_{r+2}(i_1,\ldots,i_p)}{D_{r+1}(i_1,\ldots,i_p)}$$

and

$$\max\frac{D_{r+1}(i_1,\ldots,i_p)}{D_r(i_1,\ldots,i_p)} > \max\frac{D_{r+2}(i_1,\ldots,i_p)}{D_{r+1}(i_1,\ldots,i_p)},$$

where in each case $1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n$.

Proof. We can write, as before

$$\frac{D_{r+2}(i_1,i_2,\ldots,i_p)}{D_{r+1}(i_1,i_2,\ldots,i_p)} = \frac{\sum_{T_j} A\begin{pmatrix} i_1,i_2,\ldots,i_p \\ j_1,j_2,\ldots,j_p\end{pmatrix} D_{r+1}(j_1,j_2,\ldots,j_p)}{\sum_{T_j} A\begin{pmatrix} i_1,i_2,\ldots,i_p \\ j_1,j_2,\ldots,j_p\end{pmatrix} D_r(j_1,j_2,\ldots,j_p)}$$

$$= \frac{\sum_{T_j} A\begin{pmatrix} i_1,\ldots,i_p \\ j_1,\ldots,j_p\end{pmatrix} D_r(j_1,\ldots,j_p)\cdot\frac{D_{r+1}}{D_r}(j_1,\ldots,j_p)}{\sum_{T_j} A\begin{pmatrix} i_1,\ldots,i_p \\ j_1,\ldots,j_p\end{pmatrix} D_r(j_1,\ldots,j_p)}.$$

Hence by the generalized arithmetic mean we have for $1 \leqslant i_1 < \cdots < i_p \leqslant n$,

$$\min_{T_j} \frac{D_{r+1}}{D_r}(j_1,\ldots,j_p) < \frac{D_{r+2}}{D_{r+1}}(i_1,i_2,\ldots,i_p) < \max_{T_j} \frac{D_{r+1}}{D_r}(j_1,j_2,\ldots,j_p),$$

and the results follow. ∎

Corollary.

$$\frac{D_{r+1}}{D_r}(1,\ldots,p) < \frac{D_{r+2}}{D_{r+1}}(1,\ldots,p) < \lambda_1\lambda_2\cdots\lambda_p$$

$$< \frac{D_{r+2}}{D_{r+1}}(1,\ldots,p) < \frac{D_{r+1}}{D_r}(1,\ldots,p).$$

Proof. It is sufficient to remark that in the proof of Lemma 4 it was shown that the extreme values of $\dfrac{D_{r+1}}{D_r}(i_1,i_2,\ldots,i_p)$ occurred at the end points. ∎

The final consideration in this part is the calculation of the eigenvectors of the matrix. It is natural to ask if it is possible to devise a scheme similar to the above. To this end write

$$\mathbf{g}_r = \sum_{s=1}^{n} p_s\lambda_s^r\mathbf{u}_s,$$

which can be written as

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ \lambda_1 & \lambda_2 & \cdots & \lambda_n \\ \vdots & \vdots & & \vdots \\ \lambda_1^{n-1} & \lambda_2^{n-1} & \cdots & \lambda_n^{n-1} \end{bmatrix} \begin{bmatrix} p_1\mathbf{u}_1 \\ p_2\mathbf{u}_2 \\ \vdots \\ p_n\mathbf{u}_n \end{bmatrix} = \begin{bmatrix} \mathbf{g}_0 \\ \mathbf{g}_1 \\ \vdots \\ \mathbf{g}_{n-1} \end{bmatrix}.$$

This set of equations can be solved to give

$$a_s\mathbf{u}_s = (A - \lambda_s I)^{-1}\frac{p(A)}{p'(\lambda_s)}\mathbf{g}_0,$$

where p is the characteristic polynomial of A. Hence, since we can remove any factor, we have for $s = 1, 2, \ldots, n$

$$\begin{aligned} \mathbf{u}_s &= (A - \lambda_s I)^{-1} p(A) \mathbf{g}_0 \\ &= (A - \lambda_1 I) \cdots (A - \lambda_{s-1} I)(A - \lambda_{s+1} I) \cdots (A - \lambda_n I) \mathbf{g}_0. \end{aligned}$$

This is in fact Richardson's method, which Wilkinson [11] reports to be disappointing in practice. In conclusion we remark that the schemes given above are also not stable in practice. The normal QD algorithm can be made stable by a suitable rearrangement of the table. This is possible however only because the coefficients of the polynomial for which the zeros are required is known. There does not seem to be any means of rearranging the methods given here to provide stable calculations.

4. THE COMPANION MATRIX

We turn now to the second problem, which is that of calculating the zeros of the polynomial

$$z^n + a_1 z^{n-1} + \cdots + a_{n-1} z + a_n$$

by calculating the eigenvalues of one of its companion matrices. There are four of these, and we shall confine our attention to C, the one given by

$$C = \begin{bmatrix} -a_1 & -a_2 & \cdots & -a_{n-1} & -a_n \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}. \tag{4.1}$$

It is not difficult to show that if the power method is used to find the dominant eigenvalue of C with the starting vector $[1 \ 0 \ \cdots \ 0]^T$, then the sequence of approximations to this eigenvalue is identical with the sequence which arises in Bernoulli's method as described in the introduction. Since the QD algorithm is a generalization of Bernoulli's method, it is natural to ask if there is an appropriate generalization of the power method which will give sequences which are closely connected to those generated by the QD algorithm.

It seems that treppeniteration is such a generalization; for details concerning this see Bauer [2] or Wilkinson [11].

The method is as follows. Define sequences $L_1, L_2, \ldots$ of unit lower triangular matrices and $U_1, U_2, \ldots$ of upper triangular matrices by

$$CL_{r-1} = L_r U_r, \qquad r = 1,2,\ldots, \tag{4.2}$$

where $L_0 = I$, the unit matrix.

Then if $u_{kk}^{(r)}$ denotes the (k,k) element in U_r, it can be shown that

$$\lim_{r\to\infty} u_{kk}^{(r)} = \lambda_k. \tag{4.3}$$

It is easy to see that

$$\begin{aligned} C^r &= L_r U_r U_{r-1} \cdots U_1 \\ &= L_r \tilde{U}_r, \quad \text{say.} \end{aligned} \tag{4.4}$$

Hence

$$U_r \tilde{U}_{r-1} = \tilde{U}_r,$$

and, since the product of upper triangular matrices is also upper triangular, we have

$$u_{kk}^{(r)} = \tilde{u}_{kk}^{(r)} / \tilde{u}_{kk}^{(r-1)}. \tag{4.5}$$

Denote by $\Delta_k(C^r)$ the rth principal minor of C^r; then

$$\Delta_k(C^r) = \tilde{u}_{11}^{(r)} \cdots \tilde{u}_{kk}^{(r)}. \tag{4.6}$$

Consequently

$$\tilde{u}_{kk}^{(r)} = \Delta_k(C^r)/\Delta_{k-1}(C^r), \tag{4.7}$$

and so, from (4.5), we have the result that

$$u_{kk}^{(r)} = \frac{\Delta_k(C^r)}{\Delta_{k-1}(C^r)} \frac{\Delta_{k-1}(C^{r-1})}{\Delta_k(C^{r-1})}, \qquad k = 1,2,\ldots. \tag{4.8}$$

Lemma.

$$C^r = \begin{bmatrix} u_r & u_{r+1} & \cdots & u_{r+n-1} \\ u_{r-1} & u_r & \cdots & u_{r+n-2} \\ \vdots & \vdots & & \vdots \\ u_{r-n+1} & u_{r+n-2} & \cdots & u_r \end{bmatrix}$$

$$\times \begin{bmatrix} 1 & a_1 & a_2 & \cdots & a_{n-1} \\ 0 & 1 & a_1 & \cdots & a_{n-2} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Proof (by induction). The elements in the first matrix satisfy the recurrence

$$u_{n+r} + a_1 u_{n+r-1} + \cdots + a_{n-1} u_{r+1} + a_n u_r = 0, \qquad r = -n+1, -n+2, \ldots,$$

where $u_0 = 1$, $u_{-1} = u_{-2} = \cdots = u_{-n+1} = 0$.

It is not difficult to verify that the matrix

$$\begin{bmatrix} u_0 & u_1 & \cdots & u_{n-1} \\ 0 & u_0 & \cdots & u_{n-2} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & u_0 \end{bmatrix} \begin{bmatrix} 1 & a_1 & \cdots & a_{n-1} \\ 0 & 1 & \cdots & a_{n-2} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

is in fact the identity matrix. Suppose the result is true for $r = 1, 2, \ldots, p$. Then

$$C^{p+1} = \begin{bmatrix} -a_1 & -a_2 & \cdots & -a_n \\ 1 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} u_p & u_{p+1} & \cdots & u_{p+n-1} \\ u_{p-1} & u_p & \cdots & u_{p+n-2} \\ \vdots & \vdots & & \vdots \\ u_{p-n+1} & u_{p-n+2} & \cdots & u_p \end{bmatrix}$$

$$\times \begin{bmatrix} 1 & a_1 & \cdots & a_{n-1} \\ 0 & 1 & \cdots & a_{n-2} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix},$$

but since $-a_1u_p - a_2u_{p-1} - \cdots - a_nu_{p-n+1} = u_{p+1}$ etc., it is clear that

$$C^{p+1} = \begin{bmatrix} u_{p+1} & u_{p+2} & \cdots & u_{p+n} \\ u_p & u_{p+1} & \cdots & u_{p+n-1} \\ \vdots & \vdots & & \vdots \\ u_{p-n+2} & u_{p-n+1} & \cdots & u_{p+1} \end{bmatrix}$$

$$\times \begin{bmatrix} 1 & a_1 & \cdots & a_{n-1} \\ 0 & 1 & \cdots & a_{n-2} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix},$$

which completes the induction.

COROLLARY.

(i) $\Delta_k(C^r) = (-1)^{k-1}H^{(k)}_{r-k+1}$,
(ii) $u^{(r)}_{kk} = q^{(k)}_{r-k} - e^{(k-1)}_{r-k}$.

Proof. The kth principal minor of C^r is

$$\begin{vmatrix} u_r & u_{r+1} & \cdots & u_{r+k-1} \\ u_{r-1} & u_r & \cdots & u_{r+k-2} \\ \vdots & \vdots & \cdots & \vdots \\ u_{r-k+1} & u_{r-k+2} & \cdots & u_r \end{vmatrix} \begin{vmatrix} 1 & a_1 & \cdots & a_{k-1} \\ 0 & 1 & \cdots & a_{k-2} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{vmatrix}.$$

The first determinant in this product can be rearranged to form a Hankel determinant as defined in Section 1 to give (i).

From (4.8), with the aid of (i) we have

$$u_{kk}^{(r)} = \frac{H_{r-k+1}^{(k)} H_{r-k+1}^{(k-1)}}{H_{r-k+2}^{(k-1)} H_{r-k}^{(k)}},$$

and from the definitions of $q_r^{(k)}$ and $e_r^{(k)}$ the second result follows. ∎

Thus we see that as a consequence of (ii)

$$\lim_{r\to\infty} u_{kk}^{(r)} = \lambda_k.$$

In conclusion we shall show how Rutishauser's *LR* algorithm when applied to the companion matrix is connected to his *QD* algorithm when applied to the polynomial.

The *LR* algorithm [10] is defined by the following sequence:

$$A_r = L_r R_r, \quad A_{r+1} = R_r L_r, \qquad r = 1,2,\ldots,$$

where L_r is unit lower triangular, R_r is upper triangular, and $A_1 = A$. It can be shown (see Wilkinson [11] for a detailed treatment) that if the eigenvalues are distinct, then they appear as the elements on the diagonal of R_r arranged in decreasing order as $r\to\infty$. Now it can be shown that the upper triangular matrices which occur in this and treppeniteration are in fact algebraically identical. Consequently, if the *LR* algorithm is chosen to solve the eigenvalue problem, the manner of convergence is the same as that of both treppeniteration and the *QD* algorithm.

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